Using computational approaches to investigate mechanisms of molecular motors

Lin Li

Abstract

Dynein is an important molecular motor which transports cargos along microtubules in the cell. Dysfunction of dynein leads to many serious diseases. Therefore, many efforts have been contributed to investigate the mechanisms of dynein's motilities on microtubules. However, the large size of the dynein and microtubule system makes it extremely challenging to study the atomic details of the dynein's motilities. Several computational approaches are developed and applied to study the dynein at different levels. Our simulations demonstrate that the long range electrostatic interaction plays several essential roles during dynein's motion. The electrostatic forces control dynein's binding position and orientation in each step. Meanwhile, strong evidences indicate that the electrostatic binding affinity is also a key factor to determine dynein's velocity and run length. Mutations which change the binding affinity of dynein and microtubule significantly affect dynein's velocity and run length.